

Effects of Inlet Pressure and Temperature, and Fuel-Air Equivalence Ratio on Natural Gas Combustion Utilizing the GRI Mech 3.0 Chemical Kinetics Mechanism

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Abstract

With petroleum in ever diminishing reserves and increasing demand, alternative energy sources will be of growing importance in the coming decades. Natural gas has risen as a particularly promising alternative, due to its potential to burn cleaner than petroleum and its availability as a mineable resource in the form of shale. According to the Alternative Fuels and Advanced Vehicles Data Center in the Department of Energy, there are already 13 million natural gas vehicles in operation worldwide, with about 112,000 in the United States alone. Understanding how these vehicles can be made to operate in ways that minimize emissions is of great importance. Many narrow case studies have been done to characterize the performance of natural gas combustion, but none have specifically focused on relating inlet conditions to emissions via chemical kinetic simulation. A literature review was completed in order to survey past results involving natural gas combustion in automotive applications. For this project, a methane model of natural gas combustion was simulated by utilizing CHEMKIN software and the GRI-Mech 3.0 reaction mechanism. Once the model was operational, trials were run with a varying inlet temperature, pressure, and equivalence ratio and the emissive results were observed. NO_x , CO, and CO_2 emissions were minimized at low equivalence ratio, low temperature, high pressure conditions. NO_x is defined as the sum of NO and NO_2 mol fractions.

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Table of Contents

Abstract.....	ii
Acknowledgements.....	iii
List of Figures	v
List of Tables	v
Introduction and Past Literature.....	1
Modeling Natural Gas Combustion in CHEMKIN	4
Results and Discussion	7
Minimizing Emissions.....	12
Conclusions	13
Study Limitations	14
Recommendations for Future Work	14
References	16
Appendix A: Tabulated Emission Values.....	18
Appendix B: MATLAB plotting code.....	20

List of Figures

Figure 1: Diagram View of the project setup.	5
Figure 2: Setting GRI Mech 3.0 as the reaction mechanism with accompanying thermo data.	6
Figure 3: NO _x emissions based on inlet temperature, equivalence ratio.	7
Figure 4: CO emissions based on inlet temperature, equivalence ratio.	8
Figure 5: CO ₂ emissions based on inlet temperature, equivalence ratio.	8
Figure 6: NO _x emissions based on inlet pressure, equivalence ratio.	10
Figure 7: CO emissions based on inlet pressure, equivalence ratio.	10
Figure 8: CO ₂ emissions based on inlet pressure, equivalence ratio.	11

List of Tables

Table 1: Assessment of natural gas compared to other fuels.	2
Table 2: Minimum Conditions for Emissive Species	12
Table 3: CO ₂ Emissions at Equivalence Ratio of 0.6	13

Introduction and Past Literature

The software used to model the natural gas combustion was CHEMKIN, a chemical kinetics program originally developed at Sandia National Laboratory and now managed by the company Reaction Design. At a fundamental level, combustion is governed by the rates of reacting chemicals, also known as chemical kinetics. Therefore, combustion can be effectively modeled through detailed chemical kinetics simulation software such as CHEMKIN. CHEMKIN is robust enough to handle many different types of reactions and combusting flows. In order to obtain the highest level of accuracy, a chemical reaction scheme known as GRI Mech 3.0 was utilized in this project. The GRI Mech 3.0 mechanism is named for the Gas Research Institute, a consortium that devoted a great deal of time towards developing a set of chemical reaction mechanisms specifically tailored to model natural gas combustion. GRI Mech 3.0 is based on both experimental and computational research in flame speed, ignition delay, and species profile. It consists of 325 elementary chemical reactions and associated rate coefficient expressions and thermochemical parameters for the 53 species involved. It has been optimized for reacting ranges 1000 to 2500 K, 10 Torr to 10 atm, and equivalence ratio from 0.1 to 5 for premixed systems. By implementing GRI Mech 3.0 in CHEMKIN, it was possible to develop methane model of natural gas combustion. Because emissive results were of particular interest in this project, previous studies involving natural gas combustion and emissions were reviewed extensively.

Morimoto, et al. (2001) investigated the overall effects of Exhaust Gas Recirculation (EGR) on Homogeneous Charged Compression Ignition (HCCI) natural gas combustion. Their research's primary goal was to broadly observe these effects, though power was of particular interest. The research was experimental, with measurements taken on a single-cylinder engine in a laboratory setup. EGR was found to slow combustion and lower the maximum pressure of the combustion while preserving the thermal efficiency. Emissive results were not emphasized in the study. This previous research provided a good starting point for modeling natural gas combustion. The broad appeal of natural gas as an

alternative fuel was established, with benefits in emissions mentioned. Moreover, though the emissions were not analyzed in this experiment, EGR and HCCI were established as being of particular interest for their positive effects on emissions. The temperature effect of EGR and HCCI on peak combustion temperature likely plays a role in this positive relationship.

Shanmugam, et al. (2010) conducted research comparing the performance of an engine with multiple fuels. Specifically, they investigated the performance of 10% ethanol fuel (E10), liquefied petroleum gas (LPG), and compressed natural gas (CNG). Like the previous study discussed, this research was done experimentally without any simulation component. However, this study did attempt to track and characterize the emissions resulting from each fuel. The results indicated that natural gas combustion produced significantly reduced CO and HC emissions compared not only to gasoline, but also compared to other alternative fuel options. The results are shown in Table 1.

Table 1: Assessment of natural gas compared to other fuels.

Parameter	E10	LPG	CNG
CO	-13%	-15%	-37%
HC	-19%	-39%	-45%
NOx	+16%	+38%	+44%
CO ₂	-2%	-11%	-23%
Fuel consumption	+2%	+21%	-17.5%*
Torque	-2%	-4%	-12%
Volumetric efficiency loss	Negligible	-4%	-9%
SFC (WOT)	+2%	-11%	-20%

**In terms of LGE* (Liters Gasoline Equivalent)

This study validated the necessity of further research into natural gas combustion emissions, particularly in CO and HC emissions. Though this research did characterize natural gas combustion emissions, it was different from the project because it tracked fuel effects rather than inlet conditions.

Ricklin, et al. (2002) completed a study entitled “The Effects of NO_x Addition on the Auto Ignition Behavior of Natural Gas under HCCI Conditions.” As the title implies, the research’s aim was to observe the effect of NO_x present in natural gas combustion. As before, combustion took place with HCCI. The researchers looked specifically to see if NO_x could be used to control ignition. Differing levels of NO_x (as little as 10 ppm) experimentally shifted ignition timing by several crank angle degrees, showing evidence that NO_x might be used to control natural gas HCCI ignition timing. Though emissions were specifically addressed as not being part of this study, this research did contain an aspect not found in the other papers: computational modeling based on the GRI Mech reaction mechanisms. One of the important conclusions from this paper was the assertion that chemical kinetic modeling could give qualitatively accurate results that resembled the trends seen experimentally.

Min, et al.’s (1998) study on differing natural gas fuel compositions on engine performance provided important data indicating that pure methane fuel acts similarly to natural gas fuel commercially available. The Wobber Index and maximum combustion potential of pure methane were found to be in the middle range of more complex natural gas compositions featuring ethane, propane, and nitrogen. In this way, this study validated a simplified model of pure methane for the purposes of this study.

Giang, Selamet, and Ervin’s (2002) research on the modeling of NO formation in a Perfectly Stirred Reactor (PSR) took an in-depth look at the formation and subsequent NO concentrations using CHEMKIN’s PSR. Equivalence ratio and pressure were both varied, providing somewhat similar direct benchmarks for the current study. Though the focus of the paper was comparing different models to model NO, equivalence ratio was found to have a strong effect on NO concentration, peaking near an equivalence ratio of 1.0. Pressure variations also displayed an influence on NO, with high pressures yielding a lower NO concentration at lean conditions and low pressures at rich conditions producing

lower NO concentrations. This data was quantitatively and qualitatively compared to the data from the current study.

Howes and Rideout's (1995) paper, "Evaluations of Current Natural Gas Vehicle Technology Exhaust Emissions at Various Operating Temperatures," likewise provided qualitative data with which to compare the current study's data. Four identical vehicles were made to operate on either gasoline or natural gas, with emissions closely monitored. Results varied, but generally natural gas was found to have significant reductions of non-methane hydrocarbon emissions. An important result from this study was that at lower inlet temperatures indicative of a cold start, a significant CO reduction was observed. NO_x emissions were inconsistent throughout the temperature ranges tested, with the exception of a clear, small reduction in NO_x emissions also observed at lower initial temperatures.

Though other studies have touched upon modeling natural gas combustion emissions, none have done a targeted study to examine the effects of inlet conditions on exhaust species. Furthermore, as previously discussed in this paper, the majority of current studies focus on narrowly-defined experimental measurements of particular engines. The objective of this project was to implement the GRI Mech 3.0 reaction mechanism to create a general model of natural gas combustion, map the emissions from the combustion, and study the effects of varying inlet temperature, pressure, and equivalence ratio on the observed emissions.

Modeling Natural Gas Combustion in CHEMKIN

In order to model natural gas combustion in CHEMKIN, several assumptions and simplifications had to be made. In order to model a full combustion reaction, the use of an inlet stream, perfectly-stirred reactor (PSR), and outlet flow were created. The use of an open reactor such as the PSR allowed for inlet conditions such as temperature and pressure to be modified, unlike alternative reaction

chambers such as the Internal Combustion Engine reactor and the Closed Homogeneous reactor. The project diagram used for this study can be found in Figure 1.

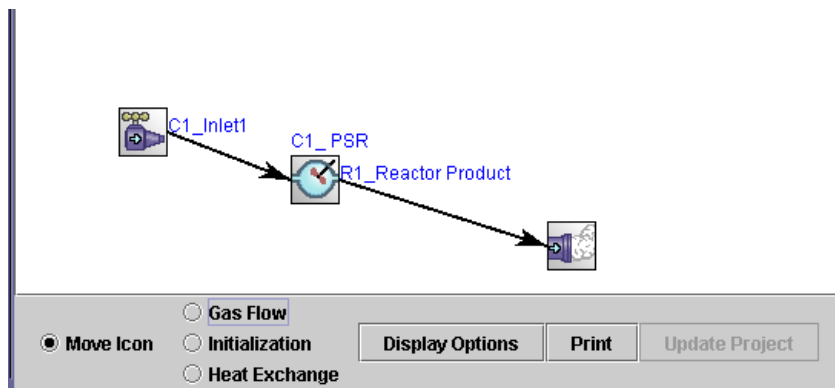


Figure 1: Diagram View of the project setup.

With the reactor, inlet, and exit specified, the next step was to specify which chemical kinetics mechanism would be applied in order to solve the combustion reaction. As referenced earlier in this paper, the GRI-Mech 3.0 was the particular mechanism of interest. GRI-Mech 3.0 also included a unique set of thermodynamic data which likewise had to be specified for this experiment. This is shown in Figure 2.

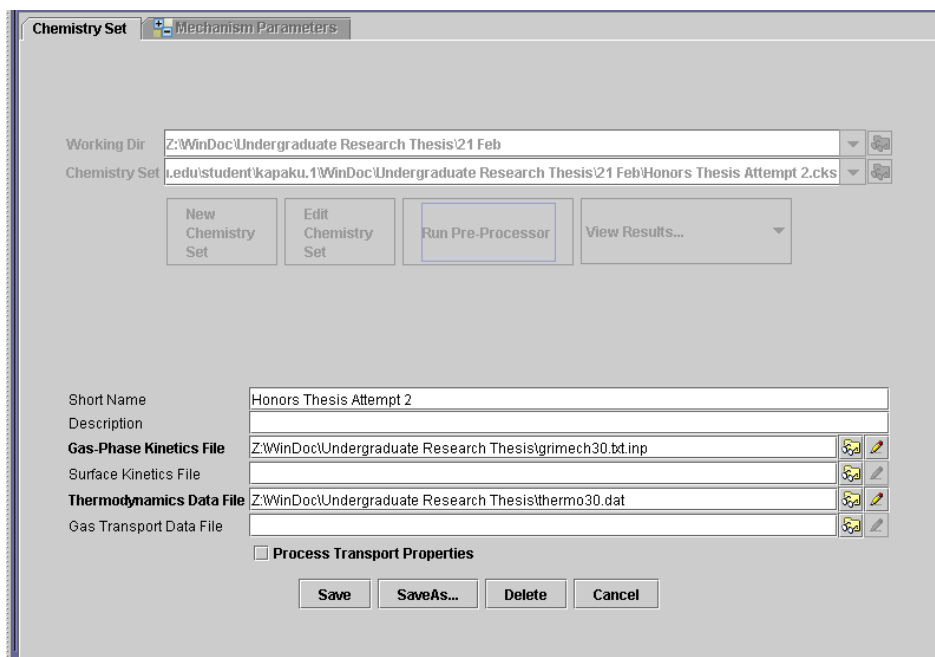


Figure 2: Setting GRI Mech 3.0 as the reaction mechanism with accompanying thermo data.

Natural gas is composed primarily of methane. In order to conduct this study, natural gas was modeled as pure methane, CH_4 . This approach was validated by Min et al., who found that pure methane acted similarly to various mixtures of natural gas. Furthermore, Min et al. acknowledged that the precise composition of natural gas varies by region, source, and processing. Though this simplification is valid, it is worth noting that real-world natural gas fuels often contain small amounts of ethane (C_2H_6), propane (C_3H_8), and nitrogen as an inert gas.

The residence time for the PSR was set to 10ms. This is a residence time chosen to coincide with the study by Giang et al. (2002) and is indicative of combustion processes that do not have time to move completely to equilibrium, such as those found in internal combustion engines. The pure methane was made to mix with air modeled as 0.79 N_2 and .21 O_2 by mol fraction. Pressure, temperature, and equivalence ratio were set as the varying parameters. The pressure range spanned 1, 5, and 10 atm. The inlet temperature range covered 298, 500, and 700K. Finally, equivalence ratio was made to vary from .6 to 1.4 in increments of .1. In all, this made for 81 unique combinations of varying parameters.

Results and Discussion

Figures 3, 4, and 5 illustrate the effects of varying inlet temperature on each emissive species.

At test conditions where the equivalence ratio was set to 1, the percent difference from the mean of the extremes was also calculated. This was done in order to highlight the actual impact of each parameter, particularly in cases where the scale of the data in the overall test range did not adequately convey the parameter's impact.

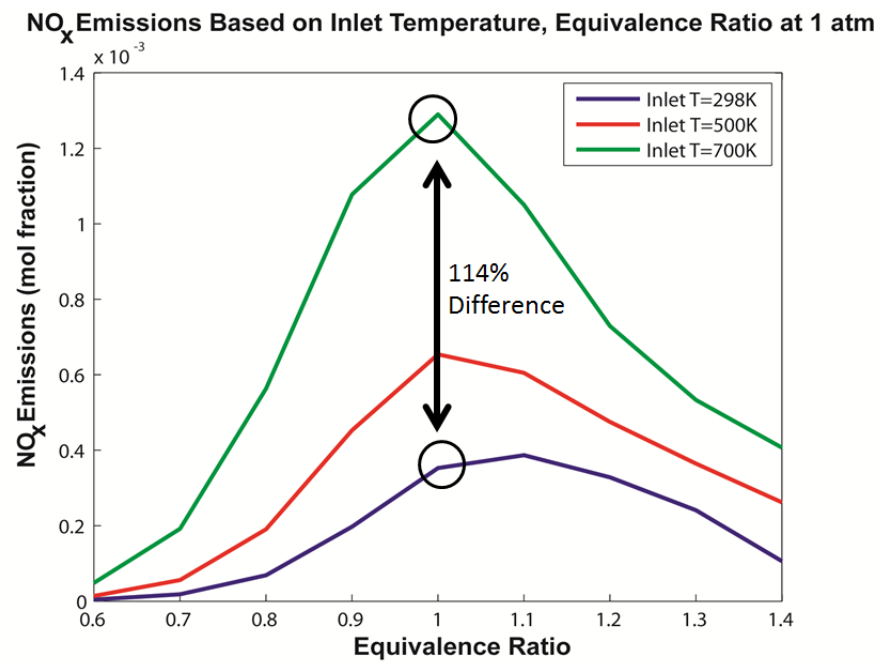


Figure 3: NO_x emissions based on inlet temperature, equivalence ratio.

CO Emissions Based on Inlet Temperature, Equivalence Ratio at 1 atm

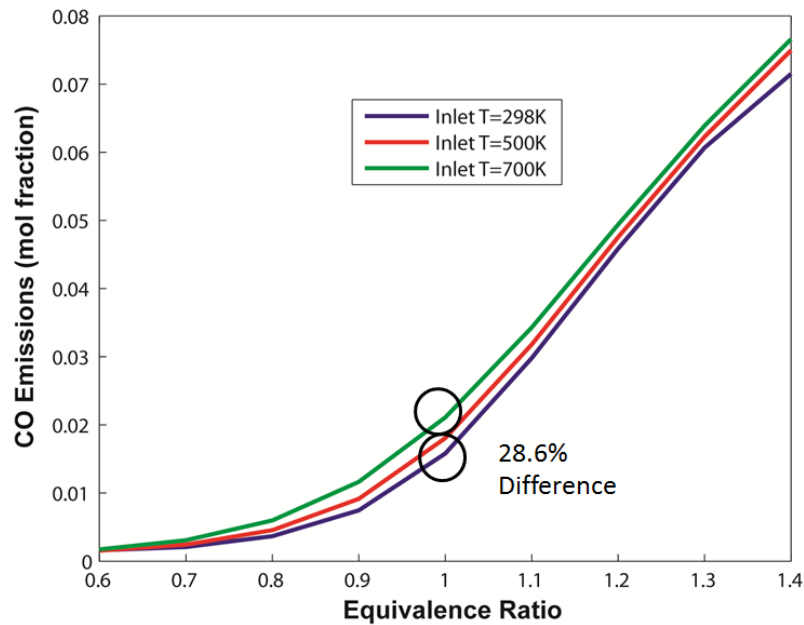


Figure 4: CO emissions based on inlet temperature, equivalence ratio.

CO₂ Emissions Based on Inlet Temperature, Equivalence Ratio at 1 atm

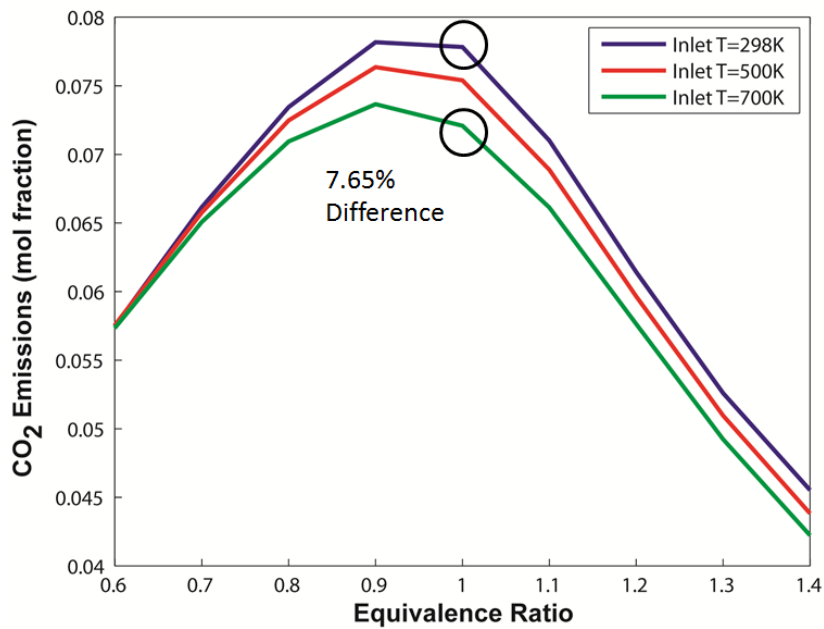


Figure 5: CO₂ emissions based on inlet temperature, equivalence ratio.

The greatest effect from temperature variation was found in NO_x emissions. This is consistent with Morimoto et al.'s (2001) and Ricklin et al.'s (2002) respective papers in the sense that they

performed experiments with EGR which indirectly would reduce the peak combustion temperature and observed noticeable deviations in results. Additionally, the lowest NO_x and CO emissions were found at the lowest inlet temperature, a result entirely consistent with Howes and Rideout's (1995) study which found that natural gas vehicles saw the greatest reduction in both CO and NO_x emissions at lower inlet temperatures. Interestingly, CO_2 emissions appeared to have the opposite trend, with the lowest CO_2 emissions corresponding to the highest temperature. No literature could be found to discuss why this may have been the case.

NO_x and CO_2 emissions both appeared to peak near an equivalence ratio of 1, while CO emissions increased as equivalence ratio increased. NO_x and CO_2 emissions fell off considerably at both high and low equivalence ratios, though NO_x had the lowest mole fraction at the lowest equivalence ratio while the lowest CO_2 mole fraction occurred at the highest equivalence ratio. It is also important to note that at either extreme of equivalence ratio, the effect of varying temperature was reduced. This was most evident at the lowest equivalence ratio of

The effects on emissive species of varying inlet pressure and equivalence ratio have been illustrated in Figures 6, 7, and 8. As before, the percent differences of the extreme values at equivalence ratio of 1 have been calculated and directly indicated on the figures.

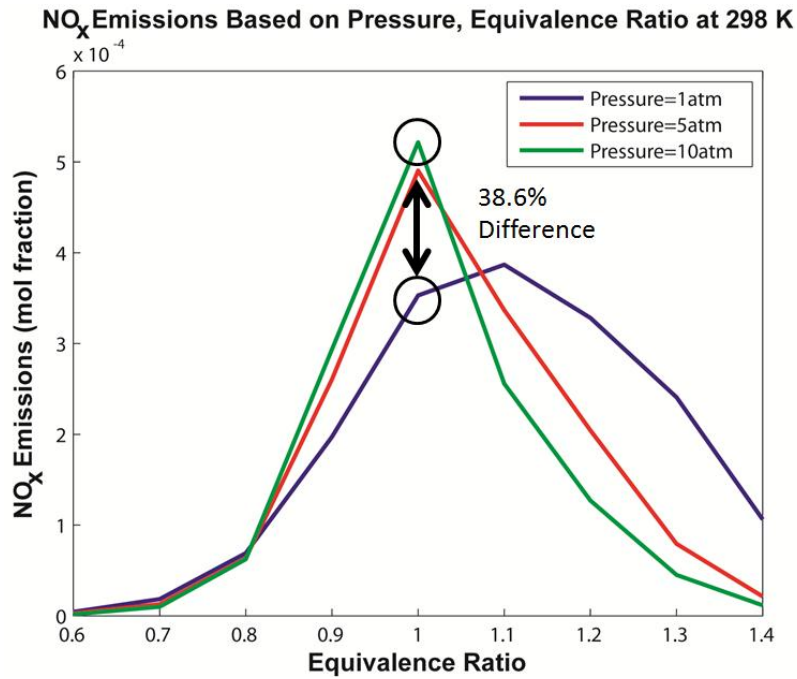


Figure 6: NO_x emissions based on inlet pressure, equivalence ratio.

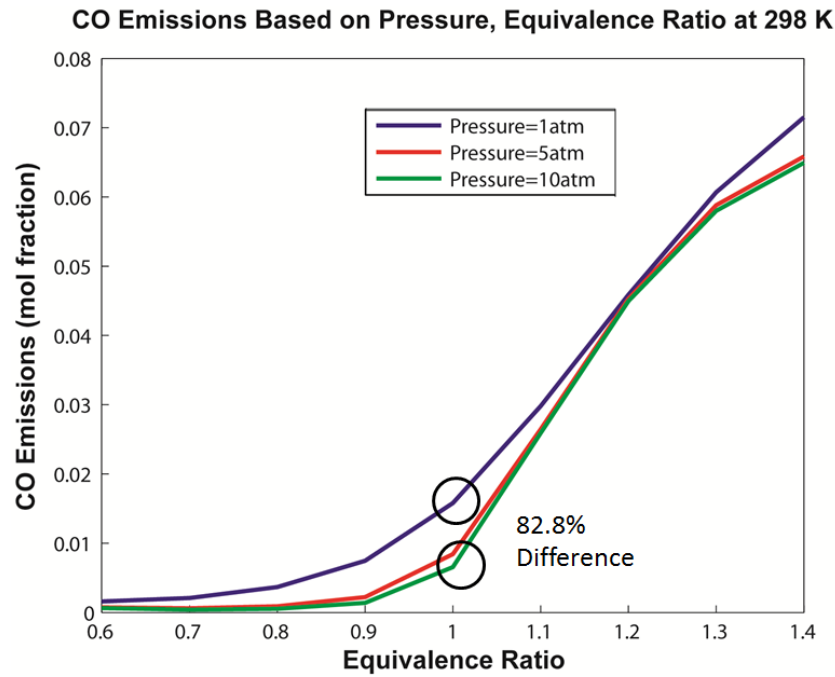


Figure 7: CO emissions based on inlet pressure, equivalence ratio.

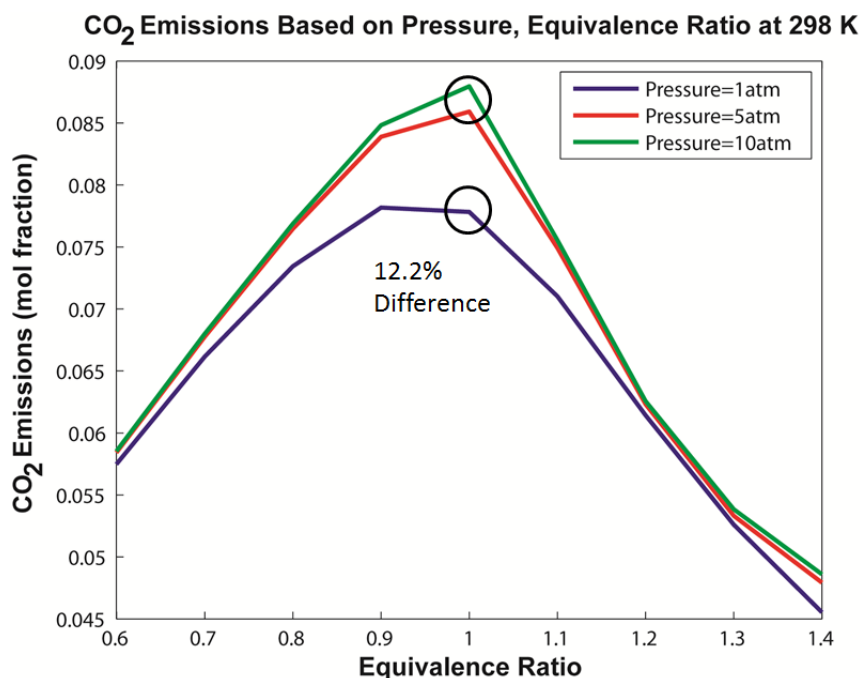


Figure 8: CO₂ emissions based on inlet pressure, equivalence ratio.

NO_x formation shown in Figure 2.6 agrees both quantitatively and qualitatively with Giang et al. (2002). That is, the mole fractions are of the same order of magnitude and the shapes of the emission curves are similar with respect to pressure and equivalence ratio. Pressure appears to play very little role in determining NO_x emissions for very lean conditions, peaking with high pressure near an equivalence ratio of 1, and then inverting with low pressure producing more NO_x emissions for rich equivalence ratios. This experiment's simulation produced peak NO_x emissions between 400 and 500 ppm, a quantitative result also seen with Giang et al. (2002).

CO and CO₂ emissions showed moderate dependence with inlet pressure. The CO did display a large percent difference at an equivalence ratio of 1, this difference was still minor compared to equivalence ratio from extreme to extreme. As with the temperature study, CO increased as equivalence ratio increased, while CO₂ peaked at or near an equivalence ratio of 1.

Minimizing Emissions

Though the focus of this study was diagnostic in nature, it is worth noting that any practical application of this data would likely revolve around minimizing harmful emissions from natural gas combustion. Therefore, now that emissive profiles with respect to inlet temperature, inlet pressure, and equivalence ratio have been created, it is possible to determine at which condition the emissions would be minimized. Table 2 contains the minimum values and corresponding conditions for each emissive specie.

Table 2: Minimum Conditions for Emissive Species

	Mol Fraction	Pressure (atm)	Temperature (K)	Equivalence Ratio
NO _x	0.000001710	10	298	0.6
CO	0.000413867	10	298	0.7
CO ₂	0.042234590	1	700	1.4

Based on these results, it would be impossible to pick a single particular condition of inlet temperature, inlet pressure, and equivalence ratio that would truly minimize all three species. While NO_x and CO follow the same trends, CO₂ appears to trend in the opposite direction. However, by inspecting Figures 5 and 8 once more, it becomes clear that CO₂ emissions are still reduced at a low equivalence ratio. Though not completely minimized, CO₂ reduction would still be beneficial for any real natural gas combustion application. Moreover, it is evident that at a lean equivalence ratio of 0.6, CO₂ mol fraction emissions become weakly associated with pressure and temperature, effectively negating their opposite trend from NO_x and CO. Table 3 demonstrates the weak pressure and temperature effects on CO₂ emissions at a lean equivalence ratio of 0.6.

Table 3: CO₂ Emissions at Equivalence Ratio of 0.6

CO ₂ Emissions at Equivalence Ratio = 0.6			
T = 298 K		P = 1 atm	
Pressure	Mol Fraction	Temperature	Mol Fraction
1 atm	0.057479600	298 K	0.057479600
5 atm	0.058413430	500 K	0.057550440
10 atm	0.058537340	700 K	0.057340930

Table 3 enables pressure and temperature to be treated as negligible parameters of influence for CO₂ at an equivalence ratio of 0.6. Combining this result with the previously-discussed result of CO₂ emissions being reduced at the low equivalence ratio, it is possible to conclude that in order to reduce NO_x, CO, and CO₂ emissions collectively, the ideal conditions would be an equivalence ratio of 0.6, a high inlet pressure of 10 atm, and a low inlet temperature of 298 K.

Conclusions

The objective of this study was to observe the effects of varying inlet temperature, pressure, and equivalence ratio on NO_x, CO, and CO₂ emissions. Utilizing CHEMKIN's PSR with the GRI Mech 3.0, the following conclusions were reached.

1. NO_x, CO, and CO₂ emissions are all strongly dependent on equivalence ratio. NO_x and CO₂ emissions peaked near an equivalence ratio of 1, while CO continued to increase as equivalence ratio increased. Minimum NO_x occurred at lean conditions, while minimum CO₂ occurred at rich conditions.
2. NO_x emissions also responded most dramatically to varying pressures and temperatures. NO_x is greatly reduced by lowering the peak combustion temperature, observed in this study by reduced inlet temperature. This behavior is consistent with published research documenting EGR, which also lowers the peak combustion temperature and reduced NO_x emissions.

3. CO emissions responded the least to temperature and pressure variations, remaining strong functions of only equivalence ratio.
4. CO₂ emissions were only moderately affected by temperature and pressure variations, minimizing at high temperature, low pressure conditions.
5. The optimal collective minimization of NO_x, CO, and CO₂ emissions occurred at a low equivalence ratio of 0.6, a high inlet pressure of 10 atm, and a low inlet temperature of 289 K.

Study Limitations

There are several important limitations to this study that must be considered when reviewing the results and conclusions. First, while conditions for minimal emissions were found, power and performance would have to be considered before any engine designs should begin. For example, a very lean equivalence ratio would decrease emissions, but would also put very little power out. It is also important to acknowledge that low temperature and lean equivalence ratio would be difficult to ignite, an effect not accounted for in this study. More work studying inlet pressure, temperature, and fuel-air equivalence ratio and their effects on power, performance, and ignition should be completed and taken with the results of this study to begin optimal natural gas engine design.

Recommendations for Future Work

There are several promising directions that future research could take, utilizing this study as a starting point. First, increased resolution over the same range of parameters could be achieved. That is, the step sizes between each parameter for each test condition could be reduced. Moreover, the limits of the parameters could be expanded in order to create a more robust emission map. The complete tabulated results could also be investigated in order to track other emissions of interest such as unburned hydrocarbons or pure nitrous oxide, NO. The model could also be refined to look at natural gas structures more complicated than simple methane. The model would also be improved with the

addition of new engine technologies such as Homogenous Charge Compression Ignition or Exhaust Gas Recirculation. Studies mentioned in the Limitations section could also improve the utility of this research. Finally, the experimental studies could be conducted to compare the calculated results to in order to apply this study to aid in the development of natural gas internal combustion engines.

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Appendix A: Tabulated Emission Values.

Table A.1: NO_x emissions based on inlet temperature, equivalence ratio.

Equivalence Ratio	NO _x (mol fraction) @ 1 atm		
	T = 298 K	T = 500 K	T = 700 K
0.6	0.000004398	0.000013668	0.000048602
0.7	0.000018463	0.000056010	0.000192153
0.8	0.000069092	0.000190891	0.000563373
0.9	0.000197321	0.000453038	0.001077759
1	0.000353076	0.000654303	0.001289709
1.1	0.000386876	0.000605177	0.001050296
1.2	0.000328160	0.000475183	0.000729131
1.3	0.000240881	0.000364784	0.000533248
1.4	0.000106221	0.000261812	0.000407093

Table A.2: CO emissions based on inlet temperature, equivalence ratio.

Equivalence Ratio	CO (mol fraction) @ 1 atm		
	T = 298 K	T = 500 K	T = 700 K
0.6	0.001593575	0.001538511	0.001734570
0.7	0.002080299	0.002440712	0.003076760
0.8	0.003671076	0.004568221	0.005989070
0.9	0.007473711	0.009162377	0.011650360
1	0.015805900	0.018052250	0.021087440
1.1	0.029806100	0.031788640	0.034294030
1.2	0.045878030	0.047555680	0.049402030
1.3	0.060673450	0.062273120	0.063889720
1.4	0.071484990	0.074955310	0.076581520

Table A.3: CO₂ emissions based on inlet temperature, equivalence ratio.

Equivalence Ratio	CO ₂ (mol fraction) @ 1 atm		
	T = 298 K	T = 500 K	T = 700 K
0.6	0.057479600	0.057550440	0.057340930
0.7	0.066151900	0.065765630	0.065077860
0.8	0.073445230	0.072477690	0.070940790
0.9	0.078175810	0.076353370	0.073657890
1	0.077822310	0.075393020	0.072087010
1.1	0.071014860	0.068874350	0.066127060
1.2	0.061430560	0.059646920	0.057633330
1.3	0.052601290	0.050965510	0.049240350
1.4	0.045537370	0.043836000	0.042234590

Table A.4: NO_x emissions based on inlet pressure, equivalence ratio.

Equivalence Ratio	NO _x (mol fraction) @ 298 K		
	P = 1 atm	P = 5 atm	P = 10 atm
0.6	0.000004398	0.000002902	0.000001710
0.7	0.000018463	0.000012793	0.000010027
0.8	0.000069092	0.000063678	0.000062595
0.9	0.000197321	0.000260763	0.000294054
1	0.000353076	0.000490731	0.000521953
1.1	0.000386876	0.000336934	0.000255759
1.2	0.000328160	0.000204313	0.000127083
1.3	0.000240881	0.000079317	0.000045148
1.4	0.000106221	0.000021282	0.000011607

Table A.5: CO emissions based on inlet pressure, equivalence ratio.

Equivalence Ratio	CO (mol fraction) @ 298 K		
	P = 1 atm	P = 5 atm	P = 10 atm
0.6	0.001593575	0.000743666	0.000629679
0.7	0.002080299	0.000620435	0.000413867
0.8	0.003671076	0.000903132	0.000532836
0.9	0.007473711	0.002227287	0.001377086
1	0.015805900	0.008425716	0.006547687
1.1	0.029806100	0.026454630	0.025907560
1.2	0.045878030	0.045275050	0.044963080
1.3	0.060673450	0.058812040	0.057997170
1.4	0.071484990	0.065827740	0.064939510

Table A.6: CO₂ emissions based on inlet temperature, equivalence ratio.

Equivalence Ratio	CO ₂ (mol fraction) @ 298 K		
	P = 1 atm	P = 5 atm	P = 10 atm
0.6	0.057479600	0.058413430	0.058537340
0.7	0.066151900	0.067758800	0.067989490
0.8	0.073445230	0.076474130	0.076883220
0.9	0.078175810	0.083893140	0.084818500
1	0.077822310	0.085922320	0.087961460
1.1	0.071014860	0.074917750	0.075548700
1.2	0.061430560	0.062317210	0.062557980
1.3	0.052601290	0.053312630	0.053837570
1.4	0.045537370	0.047934650	0.048594610

Appendix B: MATLAB plotting code.

```
% Robert Kapaku
% ME 726 Combustion
% Plotting MATLAB figures from CHEMKIN results
% Assuming that all data has been imported into variable "data"

eqrat=.6:.1:1.4;

% Show emissions cases of temp as a function of eq. ratio at 1 atm
for i=1:9
    noxplt298(i,1)=data((i-1)*9+1,9)+data((i-1)*9+1,12);
    noxplt500(i,1)=data((i-1)*9+4,9)+data((i-1)*9+4,12);
    noxplt700(i,1)=data((i-1)*9+7,9)+data((i-1)*9+7,12);
    coplt298(i,1)=data((i-1)*9+1,7);
    coplt500(i,1)=data((i-1)*9+4,7);
    coplt700(i,1)=data((i-1)*9+7,7);
    co2plt298(i,1)=data((i-1)*9+1,8);
    co2plt500(i,1)=data((i-1)*9+4,8);
    co2plt700(i,1)=data((i-1)*9+7,8);
end
    figure, plot(eqrat,noxplt298)
    hold on
    plot(eqrat,noxplt500,'r')
    plot(eqrat,noxplt700,'g')
    title('NO_x Emissions Based on Inlet Temperature, Equivalence Ratio at 1
atm')
    ylabel('NO_x Emissions (mol fraction)')
    xlabel('Equivalence Ratio')
    legend('Inlet T=298K','Inlet T=500K','Inlet T=700K')
    figure, plot(eqrat,coplt298)
    hold on
    plot(eqrat,coplt500,'r')
    plot(eqrat,coplt700,'g')
    title('CO Emissions Based on Inlet Temperature, Equivalence Ratio at 1
atm')
    ylabel('CO Emissions (mol fraction)')
    xlabel('Equivalence Ratio')
    legend('Inlet T=298K','Inlet T=500K','Inlet T=700K')
    figure, plot(eqrat,co2plt298)
    hold on
    plot(eqrat,co2plt500,'r')
    plot(eqrat,co2plt700,'g')
    title('CO2 Emissions Based on Inlet Temperature, Equivalence Ratio at 1
atm')
    ylabel('CO2 Emissions (mol fraction)')
    xlabel('Equivalence Ratio')
    legend('Inlet T=298K','Inlet T=500K','Inlet T=700K')

% Show emissions cases of pressure as function of eq. ratio at 298 K
for i=1:9
    noxplt298(i,1)=data((i-1)*9+1,9)+data((i-1)*9+1,12);
    noxp5t298(i,1)=data((i-1)*9+2,9)+data((i-1)*9+2,12);
    noxp10t298(i,1)=data((i-1)*9+3,9)+data((i-1)*9+3,12);
    coplt298(i,1)=data((i-1)*9+1,7);
    cop5t298(i,1)=data((i-1)*9+2,7);
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cop10t298(i,1)=data((i-1)*9+3,7);
co2p1t298(i,1)=data((i-1)*9+1,8);
co2p5t298(i,1)=data((i-1)*9+2,8);
co2p10t298(i,1)=data((i-1)*9+3,8);
end
figure, plot(eqrat,noxp1t298)
hold on
plot(eqrat,noxp5t298,'r')
plot(eqrat,noxp10t298,'g')
title('NO_x Emissions Based on Pressure, Equivalence Ratio at 298 K')
ylabel('NO_x Emissions (mol fraction)')
xlabel('Equivalence Ratio')
legend('Pressure=1atm','Pressure=5atm','Pressure=10atm')
figure, plot(eqrat,cop1t298)
hold on
plot(eqrat,cop5t298,'r')
plot(eqrat,cop10t298,'g')
title('CO Emissions Based on Pressure, Equivalence Ratio at 298 K')
ylabel('CO Emissions (mol fraction)')
xlabel('Equivalence Ratio')
legend('Pressure=1atm','Pressure=5atm','Pressure=10atm')
figure, plot(eqrat,co2p1t298)
hold on
plot(eqrat,co2p5t298,'r')
plot(eqrat,co2p10t298,'g')
title('CO2 Emissions Based on Pressure, Equivalence Ratio at 298 K')
ylabel('CO2 Emissions (mol fraction)')
xlabel('Equivalence Ratio')
legend('Pressure=1atm','Pressure=5atm','Pressure=10atm')

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